



chain nodes :

7 14 15 16 17 18 19 20 21 22 23 24 25 26 27 29 30 35 36 37 38

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13

chain bonds :

6-14 7-15 9-17 14-15 14-35 15-16 16-23 17-18 17-25 18-19 18-20 20-21 20-22 24-25
25-27 25-26 35-36 36-37 36-38

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

7-15 14-35 16-23 18-19 20-21 20-22 24-25 35-36

exact bonds :

6-14 9-17 14-15 15-16 17-18 17-25 18-20 25-27 25-26 36-37 36-38

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

G1:MeO,EtO,n-PrO,i-PrO,n-BuO,i-BuO,s-BuO,t-BuO,PhO,N

G2:Ph,n-PrO,i-PrO,Cb,Cy,O

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:Atom 20:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 29:CLASS 30:CLASS 31:Atom
32:Atom 35:Atom 36:Atom 37:Atom 38:Atom